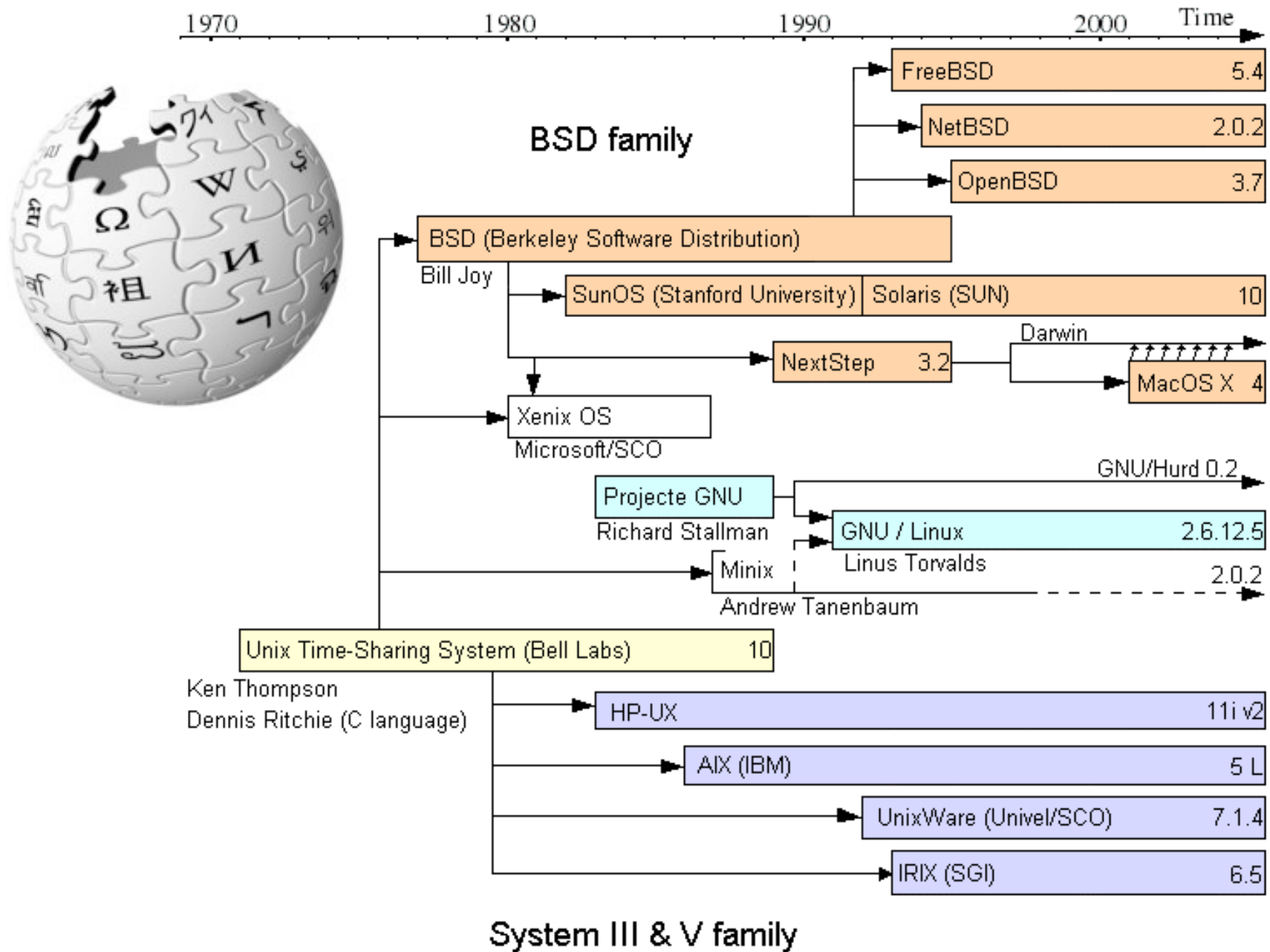
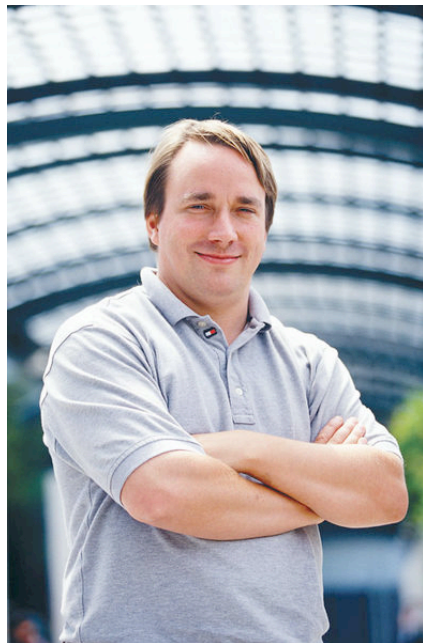
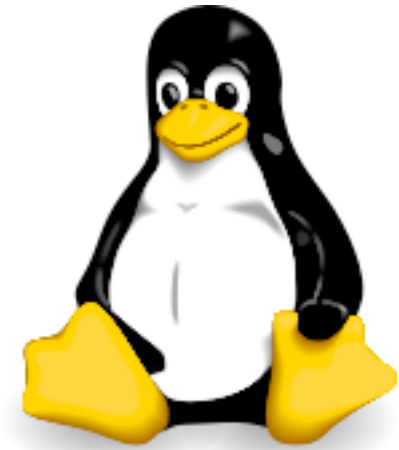


# Unix



# LINUX

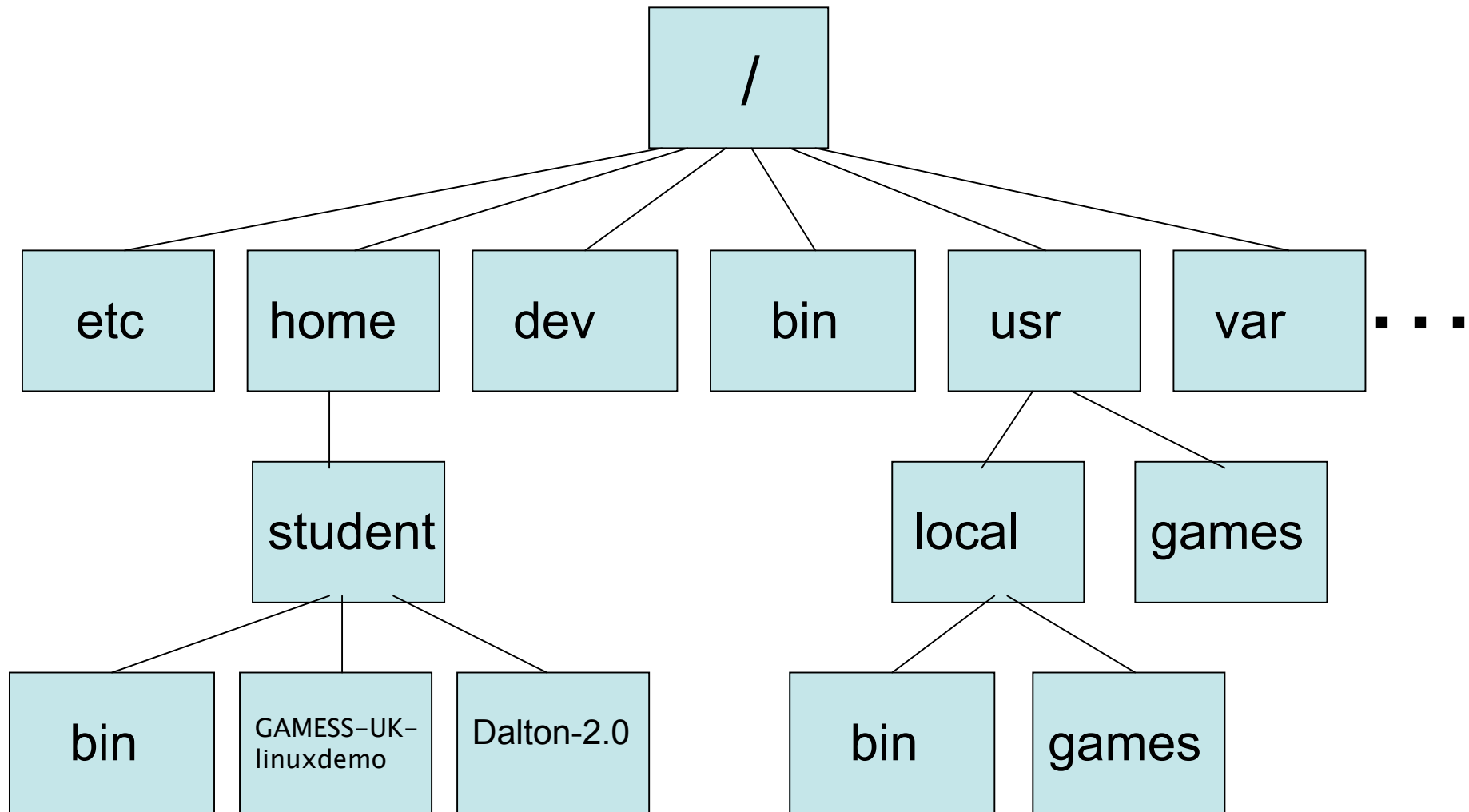
1983- **GNU**\* Project, towards a complete Unix-like operating system composed entirely of free software. 1990s, **GNU** had most of the necessary components - libraries, compilers, text editors, a **Unix**-like shell—except for the core component, the kernel. The **GNU** kernel proved difficult. \* **GNU** = **GNU**'s **N**ot **U**nix



Linus Torvalds

1991, a kernel was begun as a hobby by Finnish university student Linus Torvalds (Helsinki). Torvalds originally used **Minix**, a simplified **Unix**-like system written by Andrew Tanenbaum (Amsterdam) for teaching. Tanenbaum did not permit others to extend his operating system, leading Torvalds to create a replacement for **Minix**.

# Filesystem



Directories

# Commands (no capitals)

- **man** (-k) command : Manual -k gives list of applicable pages
- **mkdir** path : Make directory
- **ls** (-al) path : List contents of directory
- **cd** path : go to directory  
~ = your home; ../ = 1 up
- **pwd** : print working directory
- **cp** (-i) file1 file2 : copy file1 to file2
- **mv** (-i) file1 file2 : move file1 to file2
- **rm** (-i) file : remove (delete) a file or directory (-r)
- **cat** file : display a file
- **more** file : display file in pages (/ , ? Search; q quit)
- **ps** : proces status
- **grep** pattern file : display lines containing the pattern
- **name** : run a procedure or a program  
e.g. gamess,vi,molden,nedit,install.csh

# vi

# Programs-1

Unix text editor / full screen - character commands

**a** : append; **i** : insert; **o** : open new line

- finish with **ESC** -

**u** : undo ; **x** : delete character; **r** : replace character;

**R** : replace part of line (finish **ESC**); **[#]dd** : delete line(s);

**[#]yy** : put line(s) in buffer; **p** : insert buffer; **dw** : delete word;

**h** : left; **j** : down; **k** : up; **l** : right; or arrow keys

**ctrl-F** : page-down; **ctrl-B** : page up

**:q** : quit; **:x** : save + quit; **:n** : line n; **:set number** : line-number

**:[#, #]w file** : write line range for file; **:r file** : read file in

**/pattern** : search for pattern; **?pattern** : same backwards

# Programs-2

In LINUX

have a look around in your system

On CD/Stick

**GAMESS-UK** : <http://www.cfs.dl.ac.uk/docs/index.shtml>

**DALTON** : <http://www.kjemi.uio.no/software/dalton/dalton.html>

**MOLDEN** : [http://tc5.chem.uu.nl/MOLDEN\\_Manual/molden.html](http://tc5.chem.uu.nl/MOLDEN_Manual/molden.html)

Download yourself

**Nedit** :

<http://download.fedora.redhat.com/pub/fedora/linux/core/3/i386/os/Fedora/RPMS/>

# Procedures/scripts

List of commands to be executed by a SHELL

---

```
#!/bin/csh ← The shell  
ls ← The command
```

---

```
#!/bin/csh  
cat << /END > out ← redirection  
echo 'Testing 1 2 3'  
/END  
ls  
cat < out | more ← streaming  
chmod +x out ← make out executable  
out ← run out (possibly ./out)
```

---

# *Resources on Web*

tc5.chem.uu.nl

- The GAMESS-UK 6.3 User Manual and Reference Guide
- The DALTON manual
- The MOLDEN manual
  
- Terminal/werkstation Handleiding
- QuantumChemie-dictaat Hoofdstuk 7
  
- Computing for Science (CFS)
  - Examples / Tutorials

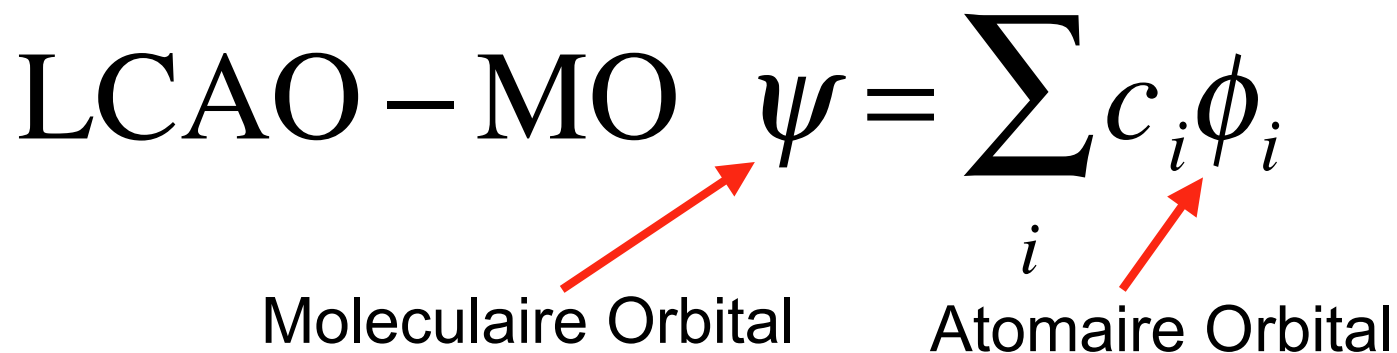
**Gaussian Basis Set Library**



# QC

LCAO – MO  $\psi = \sum_i c_i \phi_i$

Moleculaire Orbital      Atomaire Orbital



$$H = \underbrace{\sum_i \left( -\frac{1}{2} \nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} \right)}_{1\text{-electron}} + \underbrace{\sum_{A < B} \frac{Z_A Z_B}{r_{AB}}}_{\text{number}} + \underbrace{\sum_{i < j} \frac{1}{r_{ij}}}_{2\text{-electron}}$$

$$F(i) = -\frac{1}{2} \nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} + \{\text{repulsie door andere elektronen}\}$$

**Hartree-Fock**

# *Voorbeeld Job*

```
#!/bin/csh
gamess <<EOF
zmat angstrom
o
h 1 r
h 1 r 2 t
variables
r 1.04
t 104
end
EOF
```

```
chmod +x h2o
h2o >& h2o.out
```

Vragen :

- Is de Energie de som van de orbital energieen ?
- zie je een 1s orbital ?
- zie je een OH binding ?
- Hoeveel AO's zijn er ?

```
probeer toe te voegen
basis sto3g   of   basis dzp
runtype optimise  of  runtype infrared
```